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During the three-year period of this project, we conducted research on the development, analysis, and application of serial and parallel adaptive computational strategies for solving transient and steady partial differential systems. Concentrating on high-order methods and adaptive approaches that combine mesh refinement and coarsening (h-refinement, order variation (p-refinement), and occasionally, mesh motion (r-refinement), we addressed problems in combustion, materials science and compressible fluid mechanics. Special spatially-discrete finite element Galerkin methods were considered for the parallel and adaptive solution of hyperbolic conservation laws. Improved solution-limiting and error-estimation strategies increased the accuracy and efficiency of these methods which are being applied to two - and three-dimensional compressible flow problems. Adaptive techniques for dissipative systems are being applied to problems in the manufacture of ceramic composite media.

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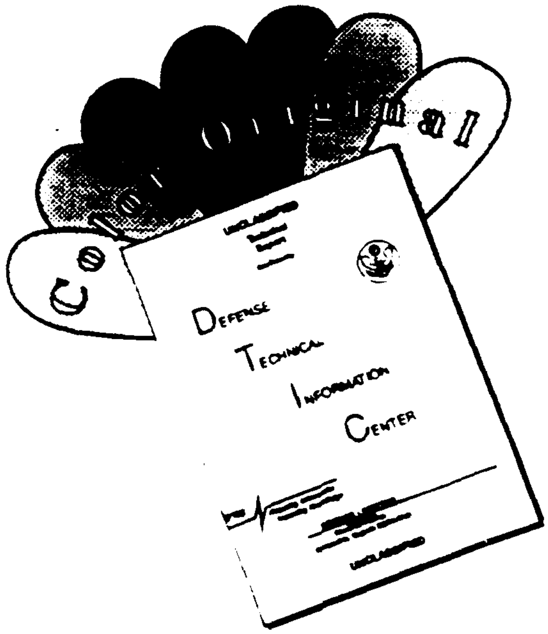

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FINAL SCIENTIFIC REPORT

Air Force Office of Scientific Research Grant AFOSR-90-0194

Period:	1 April 90 through 31 March 1993
Title of Research:	Numerical Methods for Singularly Perturbed Differential Equations with Applications
Principal Investigator:	Joseph E. Flaherty

Department of Computer Science

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ABSTRACT

During the three-year period of this project, we conducted research on the development, analysis, and application of serial and parallel adaptive computational strategies for solving transient and steady partial differential systems. Concentrating on high-order methods and adaptive approaches that combine mesh refinement and coarsening (h-refinement), order variation (p-refinement), and, occasionally, mesh motion (r-refinement), we addressed problems in combustion, materials science, and compressible fluid mechanics. Special spatially-discrete finite element Galerkin methods were considered for the parallel and adaptive solution of hyperbolic conservation laws. Improved solution-limiting and error-estimation strategies increased the accuracy and efficiency of these methods which are being applied to two- and three-dimensional compressible flow problems. Adaptive techniques for dissipative systems are being applied to problems in the manufacture of ceramic composite media.

1. Research Status and Key Results.

Research on this project involved the development, analysis, and application of adaptive finite element methods for the numerical solution of transient and steady partial differential systems. As a point of reference, consider th vector partial differential system

$$\mathbf{M}\mathbf{u}_t + \mathbf{f}(\mathbf{x},t,\mathbf{u},\nabla\mathbf{u}) = \nabla\cdot\mathbf{d}(\mathbf{x},t,\mathbf{u},\nabla\mathbf{u}),\ \mathbf{x}\in\Omega,\quad t>0. \tag{1}$$

where t denotes time, $\mathbf{x}$ denotes spatial position, ∇ is the spatial gradient or divergence operator, Ω is a bounded one-, two-, or three-dimensional region, $\mathbf{M}$ is a positive semidefinite mass matrix, and the functions $\mathbf{f}$ and $\mathbf{d}$ describe the effects of reaction, convection, and diffusion. Specific techniques aim to solve parabolic, elliptic, and hyperbolic problems that are obtained from (1) by suitable restrictions of $\mathbf{M}$ and $\mathbf{d}$.

Our concentration involved high-order methods and adaptive approaches that combined mesh refinement or coarsening (h-refinement), order variation (p-refinement), and, occasionally, mesh motion (r-refinement). The particular combination of h- and p-refinement typically produces (hp-refinement) schemes with exponential convergence rates. Temporal integration relied on either a method of lines (MOL) framework where local spatial enrichment is combined with global temporal enrichment or a local refinement method (LRM) which features local spatial and temporal enrichment. Our work on parallel adaptive strategies also concentrated on high-order techniques with the goal of developing parallel hp-refinement strategies. Given their superior performance on serial computers, consideration of other sub-optimal strategies would be dubious.

1.1. Method of Lines Techniques.

Adaptive MOL procedures utilize the power of sophisticated ordinary differential equations software and avoid the need to develop special techniques for time integration. Using the differential-algebraic systems software DASSL developed by Petzold and the DASSL implementation within the SPRINT package,[1] we studied adaptive finite element strategies and developed software for parabolic systems that combined h-, p-, and, in one dimension, r-refinement [8, 11, 12, 16, 19].[2] The two-dimensional software uses a finite quadtree structure to manage both mesh generation and refinement. An initial unstructured mesh of triangular and/or quadrilateral elements, created from terminal quadrants of the tree structure, may be further refined or coarsened by adding or deleting quadrants to or from the tree using solution-based h-refinement indicators. By modifying quadrants instead of the mesh, we maintain an underlying uniform structure while performing

[1] M. Berzins and R.M. Furzeland, "A User's Manual for SPRINT - A Versatile Software Package for Solving Systems of Algebraic, Ordinary and Partial Differential Equations: Part 1 - Algebraic and Ordinary Differential Equations," Shell Research Ltd., Thornton Research Centre, Amsterdam, 1985.

[2] Citations correspond to the publications and manuscripts listed in Section 3.

computations on an unstructured mesh.

Estimates of spatial discretization errors are obtained by a p-refinement technique using piecewise polynomial approximations of one degree higher than those used for the solution to solve local problems with forcing proportional to elemental or edge residuals. Errors of odd-degree finite element solutions are approximated using edge residuals while neglecting elemental residuals. Those of even degree solutions follow the opposite course. Error estimates computed in this manner converge in energy at the correct rate to the actual finite element spatial errors under h-refinement [11]. Our results show that this edge or elemental "superconvergence" is robust in time; hence, temporal variation of spatial errors may be neglected [11, 12]. This enables us to determine error estimates by solving local elliptic instead of local parabolic problems. The advantage of this approach is that error estimates may be computed only when needed and not at every time step selected by the ordinary differential equations software. In typical applications [8, 11, 12], this reduces the time required to obtain an error estimate by approximately thirty percent.

1.1.1. Case Study: Boundary Resonance.

The problem

$$u_t + xu_x = \varepsilon u_{xx}, \quad -1 < x < 1, \quad t > 0, \tag{2a}$$

$$u(-1,t) = 3, \quad u(1,t) = 5, \quad t > 0, \tag{2b}$$

$$u(x,0) = x + 4, \quad -1 \le x \le 1. \tag{2c}$$

is an example of boundary resonance[3] in the singularly-perturbed limit $0 < \varepsilon \ll 1$. As t increases, the smooth initial data evolves to the steady state

$$u(x) = xe^{x^2/2\varepsilon} M(1, \frac{3}{2}, -\frac{x^2}{2\varepsilon}) + 4 \tag{2d}$$

where $M(a,b,c)$ is Kummer's function. This steady solution has boundary layers of width $O(\sqrt{\varepsilon})$ at both endpoints. The problem (2), connected with exit-time probability determination, is challenging because (i) singular-perturbation theory does not suffice to determine the interior solution (i.e., the solution on $-1 < x < 1$) and (ii) the transient solution evolves to a steady state at an exponentially slow rate (i.e., in $O(e^{-1/\varepsilon})$ time).

Adjerid et al. [12, 19] computed solutions of (2) using adaptive h-, hr-, and hp-refinement with $\varepsilon = 0.001$ and several error tolerances in H^1. Integration, starting with a

[3] C. Holland, Personal communication, 1989.

ten-element mesh, was continued to $t = 20$, which was taken as steady state. The solution generated by adaptive hp-refinement with an error tolerance of 0.03 relative to $\|u\|_1$ is shown at $t = 0$ and 20 in Figure 1.

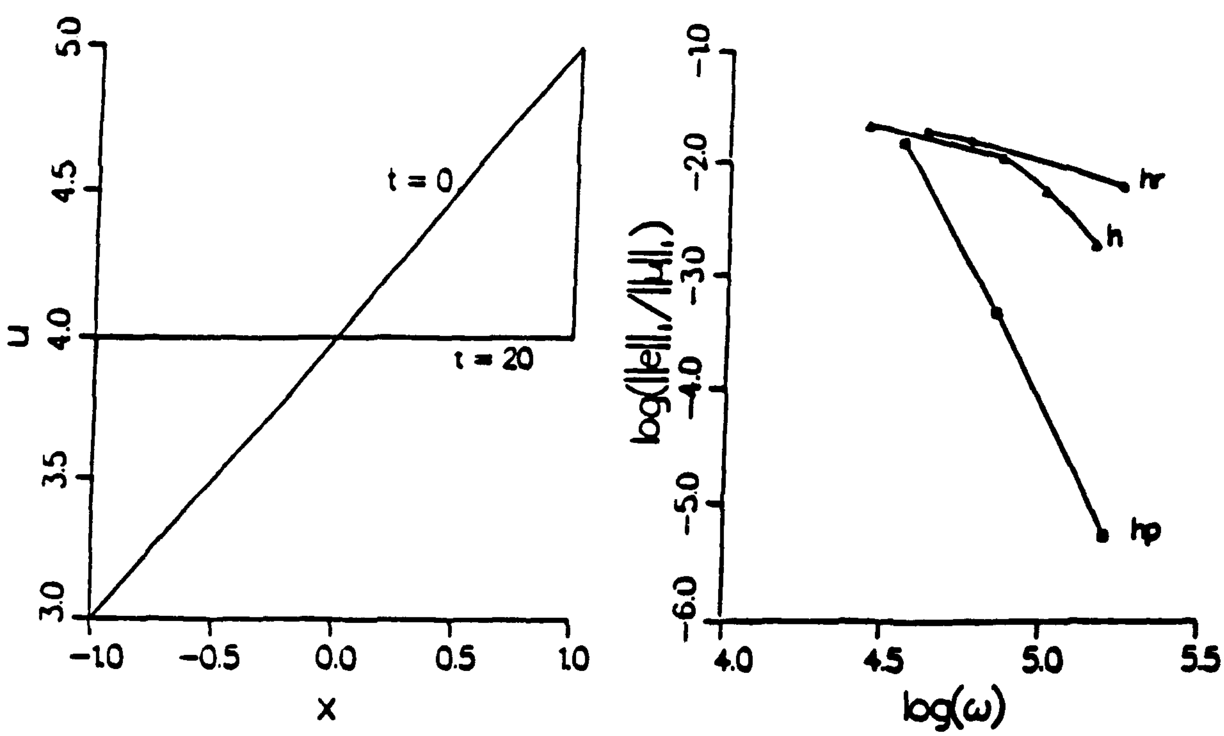

Figure 1. Finite element solution of (2) at $t = 0$ and 20 using adaptive hp-refinement with a relative tolerance of 0.03 on a 10-element initial mesh (left). Relative error as a function of work ω using adaptive h-, hr-, and hp-refinement (right).

The discretization error is shown as a function of the total work [12] ω for solutions computed by adaptive h-, hr-, and hp-refinement at the right of Figure 1. Accuracy of all methods are comparable for the larger errors, but hp-refinement is much more efficient at higher accuracy. A "warm restarting" procedure [8] enables the backward difference software within DASSL to resume the temporal integration at a high order whenever h-refinement has been performed and this has improved the performance of the h- and hp-refinement schemes and has reduced the need for mesh motion.

Consider a related two-dimensional problem[4]

[4] C. Holland, Personal communication, 1991.

$$u_t + \mathbf{f}(x,y)\cdot\nabla u = \varepsilon\Delta u, \quad (x,y)\in\Omega, \quad t > 0, \tag{3a}$$

with

$$\mathbf{f}(x,y) = [-y - x(1-r^2),\ x - y(1-r^2)]^T, \tag{3b}$$

$\Omega = \{ (x,y) \mid -2 < x < 1.5, -3 < y < 3 \}$, and $r^2 = x^2 + y^2$. With this resonance problem, the solution in the interior of the domain is determined by the data at the point(s) on the boundary that is (are) closest to the origin.

The solution shown in Figure 2 was obtained by integrating the transient parabolic problem with $\varepsilon = 0.01$ to steady state using hp-refinement with a relative error tolerance of 0.02 in H^1. Mesh refinement with relatively low-order methods occurs in boundary layers near $y = \pm 3$ and $x = 2$. The smooth solution in the interior and near $x = 1.5$ was obtained on a coarser mesh principally with p-refinement. Standard numerical techniques for solving this problem would produce non-physical oscillations unless the mesh was sufficiently fine within the boundary layers but, with hp-refinement, the solution has been captured correctly in near optimal fashion.

As a final example of resonance, consider the elliptic problem[5]

$$xu_x + yu_y = \varepsilon\Delta u, \quad (x,y)\in\Omega, \tag{4a}$$

with $\Omega = \{ (x,y) \mid -2 < x < 1, -3 < y < 3 \}$.[6] Problems (2) and (3) were solved using adaptive techniques with standard finite element-Galerkin methods. In order to reduce the dependence on proper mesh placement or sophisticated temporal embedding, we have developed special quadrature rules that produce stable numerical strategies for a variety of singularly-perturbed problems. This technique will be described in a forthcoming manuscript;[7] however, for the moment, we note that these rules are approximately Radau quadrature for this example. The solution of (4) shown in Figure 3 was obtained with $\varepsilon = 0.001$ using adaptive h-refinement on a 20×20 initial mesh with piecewise-linear approximations and the special quadrature rules. Boundary layers on the three edges that are farthest from the origin are sharp, no spurious oscillations are present, and the correct interior solution is obtained.

These resonance problems are extremely difficult. Convergence to steady state at an exponentially slow rate implies that discrete versions of steady problems, such as (4), are extremely ill conditioned. Standard and adaptive techniques must fail when ε is sufficiently small. The adaptive h- and hp-refinement strategies have enabled us to

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[5] C. Holland, Personal communication, 1989.

[7] S. Adjerid, M. Aiffa, and J.E. Flaherty, "Adaptive Numerical Procedures for Singularly-Perturbed Partial Differential Equations," *Workshop on Perturbation Methods in Physical Mathematics*, Rensselaer Polytechnic Institute, Troy, June 23-26, 1993. Manuscript in preparation.

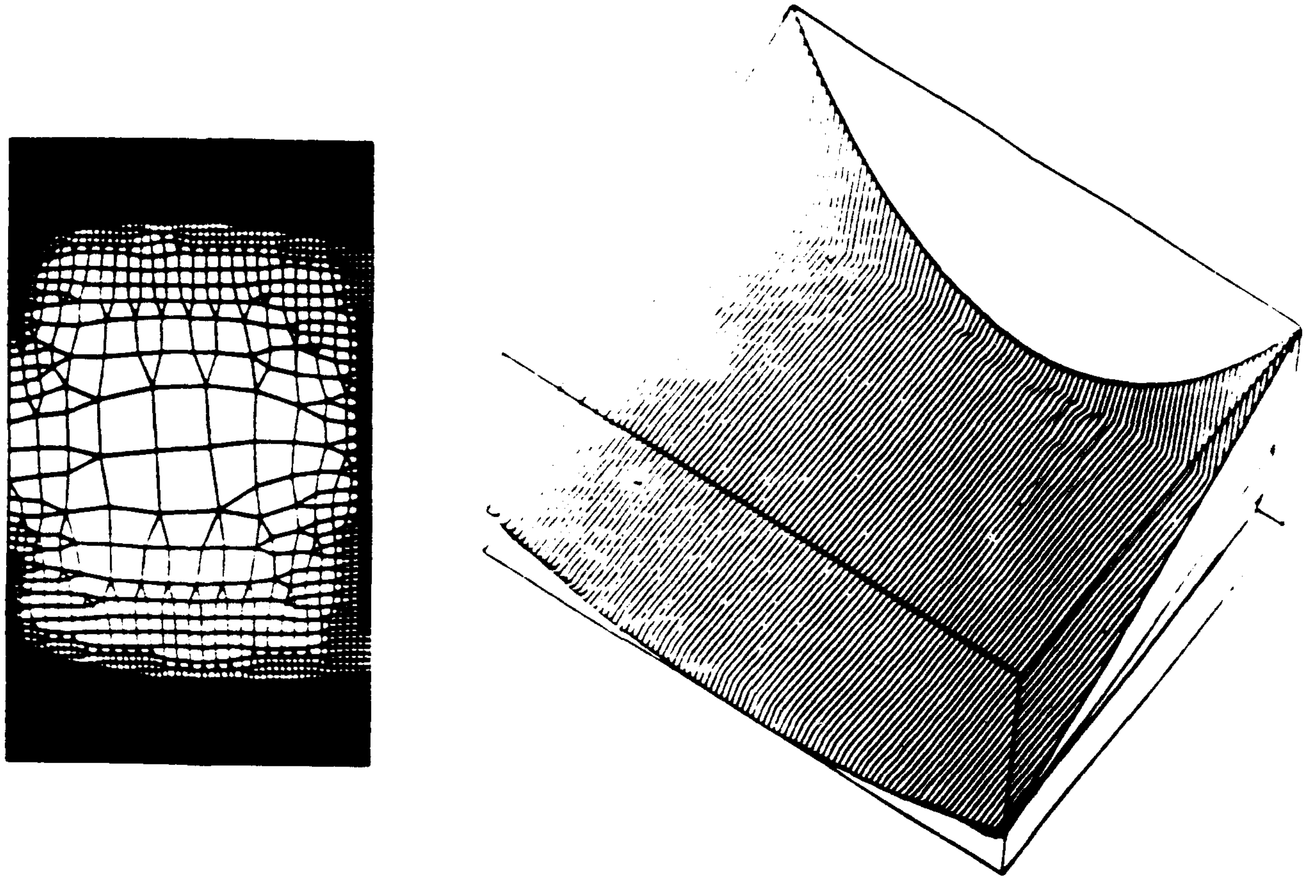

Figure 2. Mesh (left) and steady solution (right) of (3) with $\varepsilon = 0.01$ using adaptive hp-refinement.

produce solutions at smaller values of ε than would otherwise be possible. The special quadrature rules eliminate all oscillations. However, additional problem-dependent information[8] would be necessary in order to obtain solutions for very small values of ε.

1.1.2. Case Study: Materials Processing.

Working with Rensselaer Materials Scientists William Hillig, John Hudson, and Nag Patibandla, we have been using our adaptive software to study fabrication problems

[8] cf., e.g., M. Ward, "On Exponentially Slow Internal Layer Motion," *Workshop on Perturbation Methods in Physical Mathematics*, Rensselaer Polytechnic Institute, Troy, June 23-26, 1993.

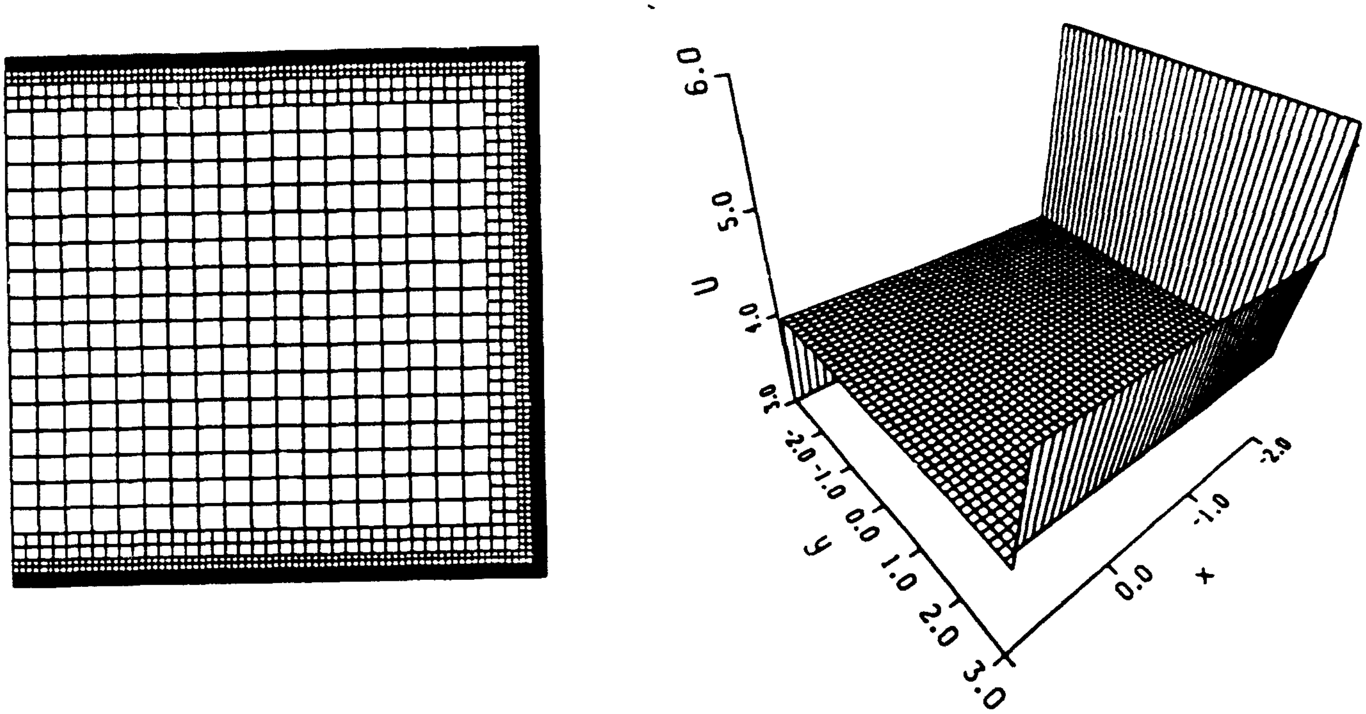

Figure 3. Mesh (left) and solution (right) of (4) with $\varepsilon = 0.001$ using adaptive h-refinement with piecewise-linear approximations on a 20×20 initial mesh and special quadrature rules.

associated with ceramic composites. The goal is to manufacture high-temperature composites having alumina (Al_2O_3) fibers and a molybdenum di-silicide ($MoSi_2$) matrix. As a preliminary study, we have been modeling the molybdenum di-silicide fabrication by a "reactive vapor infiltration" (RVI) process developed by Hillig and Patibandla. Using this process, molybdenum powder is pressed (to 45% porosity) into a pellet which is exposed at approximately $1200° C$ to a $SiCl_4$ and H_2 flow. Silicon gas is produced on the pellet's surface. It infiltrates the pellet and reacts with the molybdenum to form silicide layers of Mo_5Si_3 and $MoSi_2$. Pores between particles are filled by volume expansion as the silicides are produced and, as an initial approximation, we assumed that solid-state diffusion is the dominant means of infiltration. With this assumption, considerations of mass conservation imply

$$\frac{d}{dt}\iiint_{\Omega} \rho Y_i \, d\omega + \iint_{\partial\Omega} \mathbf{J}_i \cdot \mathbf{ds} = \iiint_{\Omega} \dot{\rho}_i \, d\omega, \quad i = 1, 2, \cdots, N, \tag{5a}$$

$$\sum_{i=1}^{N} Y_i = 1, \quad \sum_{i=1}^{N} \dot{\rho}_i = 0. \tag{5b}$$

where Y_i, $\mathbf{J}_i$, and $\dot{\rho}_i$ are, respectively, the mass fraction, flux, and production rate of species i, $i = 1, 2, \cdots, N$, and ρ is the mixture density. Assuming Fickian diffusion and first-order reactions yields the dimensionless system for the silicon-molybdenum reaction

$$\frac{\partial u_1}{\partial t} - \nabla \cdot D_1 \nabla u_1 = -(3w_1 + 7\kappa w_2), \quad \frac{\partial u_2}{\partial t} - \nabla \cdot D_2 \nabla u_2 = 5\frac{M_2}{M_1}\kappa w_2, \tag{6a,b}$$

$$\frac{\partial u_3}{\partial t} - \nabla \cdot D_3 \nabla u_3 = \frac{M_3}{M_1}(w_1 - \kappa w_2), \quad \frac{\partial u_4}{\partial t} - \nabla \cdot D_4 \nabla u_4 = -5\frac{M_4}{M_1} w_1 \tag{6c,d}$$

$$\sum_{i=1}^{4} u_i = \tilde{\rho}, \quad w_1 = u_1 u_4, \quad w_2 = u_1 u_3, \tag{6e,f,g}$$

The volume fraction u_i, diffusivity D_i, and molar mass M_i of species i, $i = 1, 2, 3, 4$, respectively, correspond to those of Si, $MoSi_2$, Mo_5Si_3, and Mo. The variable κ identifies the ratio of the production rate of $MoSi_2$ to that of Mo_5Si_3 and $\tilde{\rho}$ is the dimensionless mixture density.

We used this model with our adaptive software to solve several one- and two-dimensional problems. Results using adaptive h-refinement shown in Figures 4 and 5, respectively, exhibit the thickness of the $MoSi_2$ layer at three times and the concentrations of Si, $MoSi_2$, Mo_5Si_3, and Mo after 3.5 hours of reaction. In each drawing, high concentrations are colored red and low ones are colored blue. The mesh used for the computation at the indicated time has been superimposed. The bottom and right edges of each figure are lines of symmetry. The silicide layers progress inward from the top and left edges to build the $MOSi_2$ and Mo_5Si_3 layers. Reaction fronts are sharp and the mesh is concentrated in and following these regions. The Mo_5Si_3 layer is a narrow zone that precedes the $MoSi_2$ layer into the unreacted molybdenum.

The model and its adaptive solution correctly predicted the thickness and growth rate of the $MoSi_2$ layer to approximately 5% of measured values. Volume expansion also agreed with experimental observations. The generality of our software makes it easy to change models and include more complex and realistic effects. Recently, we were able to show that the production times of $MoSi_2$ could be reduced (potentially halved) by starting with a powder composed of a mixture of Mo, $MoSi_2$, and/or Mo_5Si_3. Hillig's and Patibandla's initial experiments are confirming these computational predictions. Since production times are approximately one day for realistic layer thicknesses, a factor of two reduction is very significant.

1.2. Local Refinement Methods.

1.2.1. Parabolic Systems.

While MOL procedures greatly simplify temporal integration, there are many situations where they would have sub-optimal performance and, for this reason, we have also been studying LRMs. A posteriori error estimates may be used to schedule different temporal and spatial enrichment strategies in different regions of the spatial domain with the possibility of providing large efficiency improvements. Given the need to interrupt the temporal integration for h-refinement more often than with a MOL procedure, one-step integration methods may be preferable to the backward difference methods that are commonly used with MOLs [2, 4]. With this possibility, we have developed a variant of the singly implicit Runge-Kutta (SIRK) method that offers several advantages when used in conjunction with hp-refinement methods for parabolic problems [18]. SIRKs have high-stage order, A-stability for orders one through eight, efficiencies close to those of backward difference software, embedded error estimates, and a locality that is suitable for parallel computation. Temporal error estimates of each SIRK stage may be computed for the cost of one additional function evaluation [18]. This permits the acceptance of solutions at partial time steps whenever accuracy is not satisfactory at the final time [25]. An adaptive hp-refinement strategy based on SIRKs and hierarchical finite element approximations is, to our knowledge, the first instance where hp-refinement has been used in both space and time [25]. Several enrichment strategies were developed and the most successful of these are being used to develop a three-dimensional solution package.

1.2.2. Hyperbolic Systems.

While hp-refinement is reasonably well understood for elliptic problems, this is far from true for time-dependent problems, particularly hyperbolic systems. Extensions of finite difference methods to higher order involve enlarging their computational stencils, which would be unsuitable for both parallel and unstructured-mesh computation. Cockburn and Shu (cf., e.g., [14, 15, 22, 24]) combine a local basis of Legendre polynomials with a solution limiting scheme to create a method that has both high order and a compact stencil. In his Rensselaer dissertation, Biswas[9] used this scheme to develop adaptive h-refinement methods for one- and two-dimensional problems. Subsequent extensions include improved projection limiting schemes near discontinuities, spatial a posteriori error estimation schemes based on p-refinement, adaptive p-refinement, and parallel solution strategies [15, 22, 24]. Spatial error estimates were computed using Radau quadrature points as described in Section 1.1.1.

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[9] Cf. the list of dissertations in Section 4.

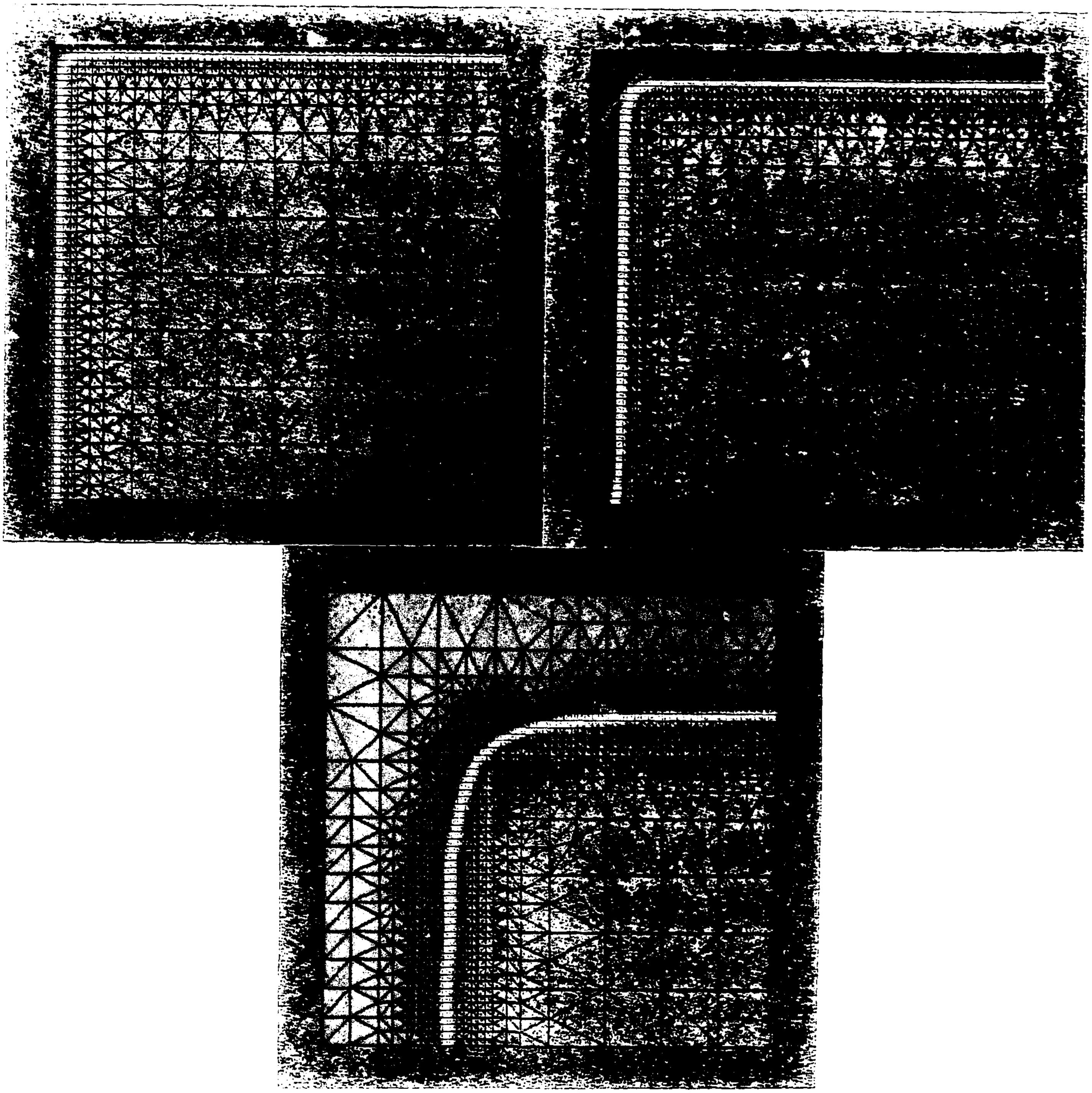

Figure 4. Volume fraction of $MoSi_2$ at 4 minutes (upper left), 21 minutes (upper right), and 3.5 hours (lower center) of reaction. High concentrations are shown in red and low concentrations in blue.

1.3. Parallel Computation.

The Construction of parallel adaptive techniques is a challenge since parallelism and adaptivity are at odds. Adaptivity employs complex heuristic decision processes that introduce serial bottlenecks and, hence, complicate parallelization. This situation is further exacerbated when unstructured grids are used as part of the computation. Nevertheless, as noted, parallelization of these most efficient techniques must be explored since parallelizing sub-optimal strategies will result in lower performance.

1.3.1. Elliptic Systems.

The need for synchronization on shared-memory computers can be reduced by constructing a list of elements that have independent basis support that may be assembled and solved in parallel. The task of separating or "coloring" the elements should be (i) computationally efficient and (ii) employ a small number of colors to maintain granularity. Algorithms to color arbitrary finite element meshes with a minimum number of colors are data and manipulation intensive; however, meshes produced by finite quadtree and finite octree procedures have a regular quadrant or octant structure that may be used to advantage. Thus, we color the quadrants or octants of the tree structure instead of the finite elements and thereby simplify the coloring process at the expense of creating a minor load imbalance due to the variation in the number of elements per quadrant or octant.

Benantar et al. [3, 6, 7, 9, 10, 17] described a six-color procedure for coloring quadtree structures that was used to solve elliptic problems with a piecewise-linear basis. Conjugate gradient iteration with element-by-element and symmetric successive over relaxation (SSOR) preconditionings were used to solve the resulting linear algebraic systems. The procedures worked well with the SSOR preconditioner providing the best performance; however, performance degraded when high-order approximations and adaptive p-refinement were added to the solution process. Since hierarchical bases of degree greater than unity involve edge- and element-level interactions, an edge coloring procedure should improve parallel performance.

Benantar, in his Rensselaer dissertation, considered edge coloring procedures for two-dimensional meshes of triangular elements. Creating a new discrete structure, called a *triangle graph*, he showed that mesh edges could be colored using a maximum of three colors by a procedure that had at most quadratic time complexity [17, 21]. Contrary to the quadrant-coloring procedure, performance improves with increasing polynomial degree; thus, this is an effective procedure for parallel p-refinement.

1.3.2. Hyperbolic Systems.

We are using the spatially discontinuous Galerkin-finite element procedure described in Section 1.2.2 to construct parallel h- and p-refinement techniques on MIMD systems for

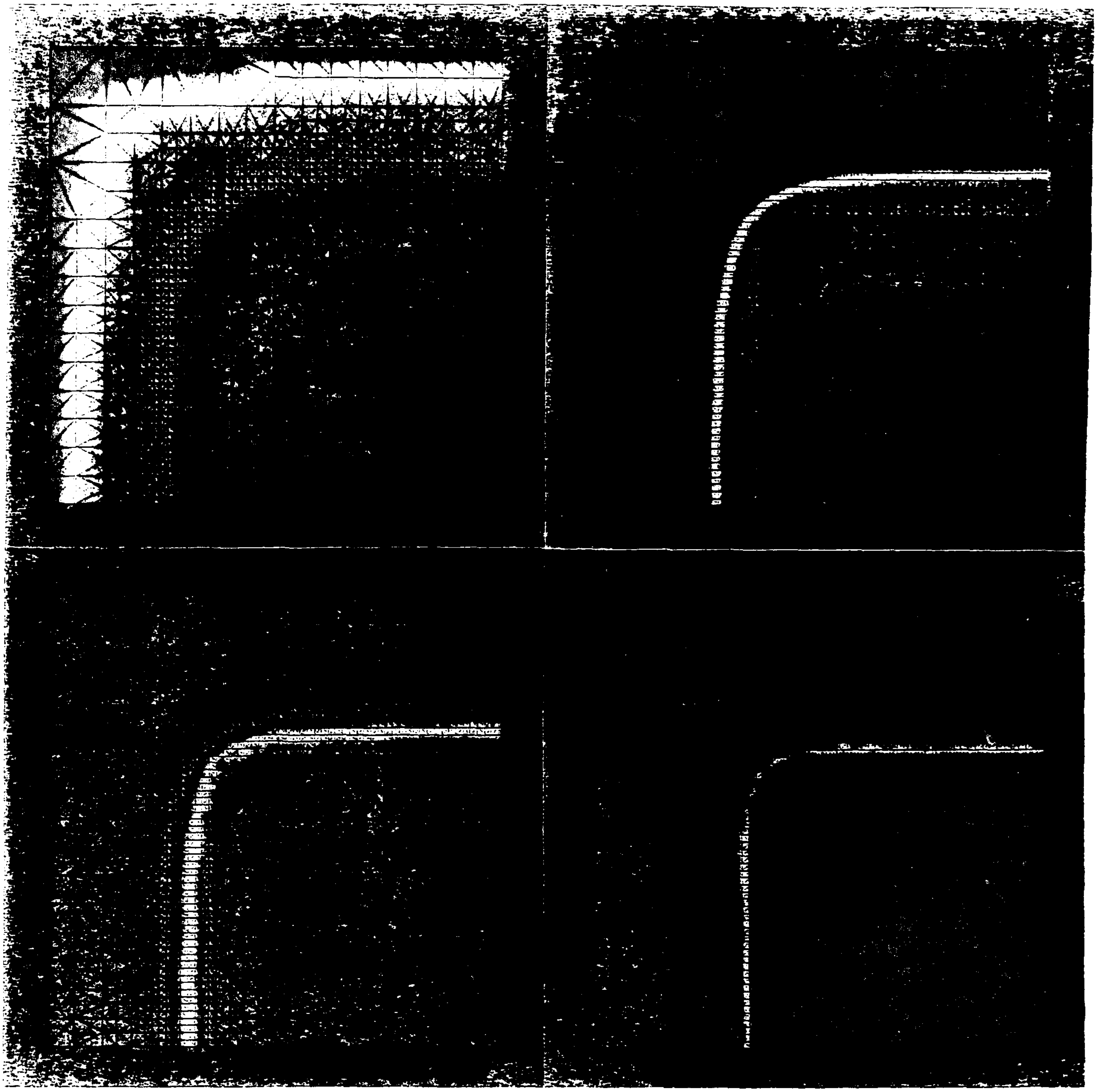

Figure 5. Volume fraction of Si (upper left), $MoSi_2$ (upper right), Mo_5Si_3 (lower left), and Mo (lower right) after 3.5 hours of reaction. High concentrations are shown in red and low concentrations in blue.

two- and three-dimensional conservation laws. The two-dimensional p-refinement software uses a tiling strategy developed by Wheat [24] to appraise neighborhood workloads and migrate elements to nearby processors as appropriate. Migration is far more efficient with adaptive computation than global optimization methods. Computational experiments using a ten-dimensional NCube 2 hypercube at Sandia National Laboratories indicated a 52 percent increase in performance with this tiling algorithm relative to no migration. We expect further performance improvements to occur by predicting future workload changes using solution and error information.

Extending the spatially discontinuous Galerkin procedure to three dimensions, we consider parallel adaptive h-refinement on octree-structured grids. An example involving the supersonic (Mach two) flow over a cone is shown in Figures 6 and 7. In Figure 6, we show the initial and final meshes used for this computation. Refined meshes were created by introducing additional octants into the tree structure and generating a new mesh locally. Steady solutions were obtained by integrating the transient Euler equations to steady state with local time steps proportional to tree level. Load balancing on a CM-5 Connection Machine was performed by a traversal of the octree structure using a work metric at each tree node. Pressure contours and the shock surface, shown in Figure 7, indicate that the mesh is being refined in the vicinity of the leading bow shock. Higher-order methods and p-refinement will be added to the method shortly.

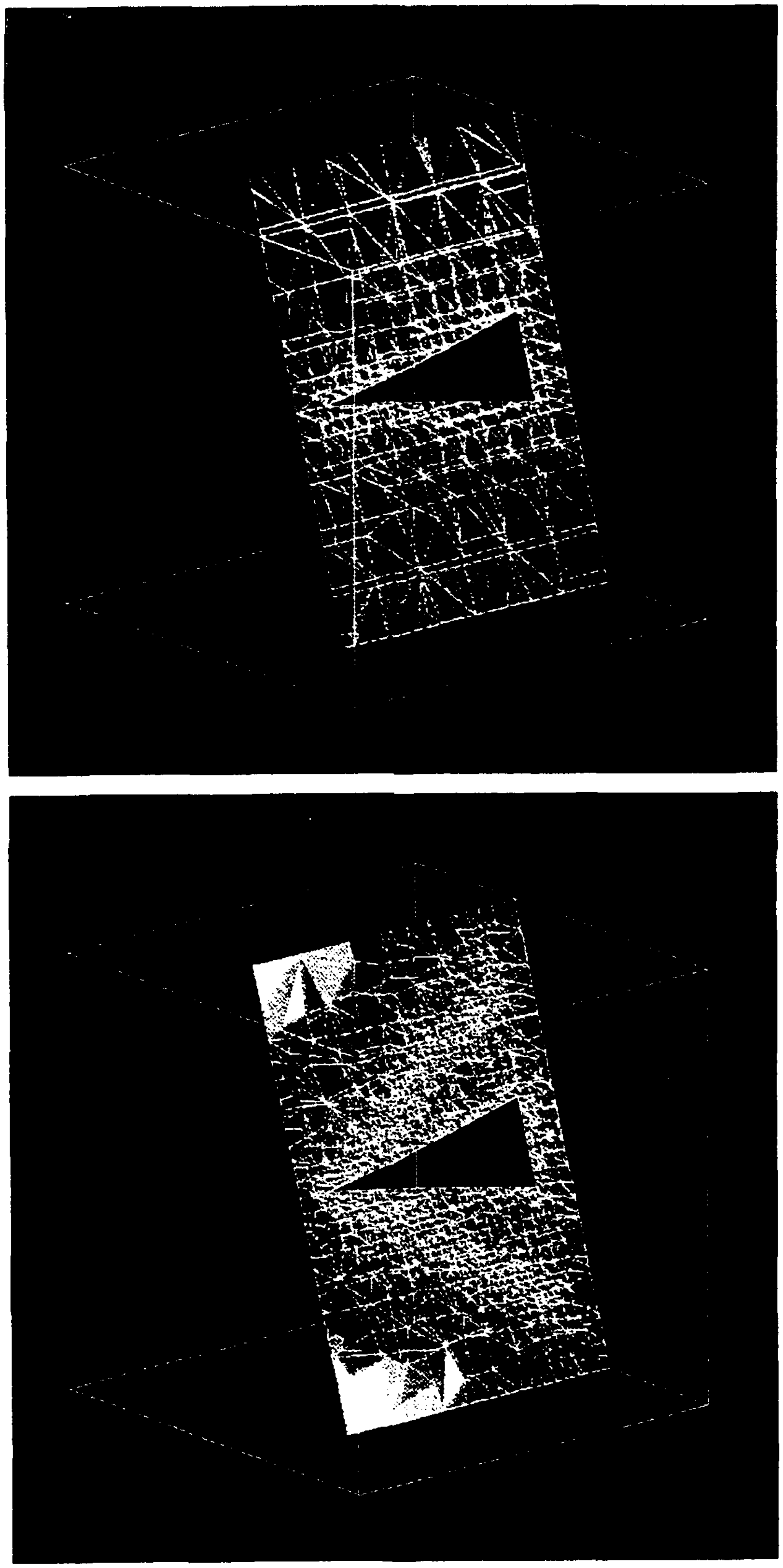

Figure 6. Coarse (top) and fine (bottom) meshes used to compute the Mach two flow past a cone having a half angle of 10°.

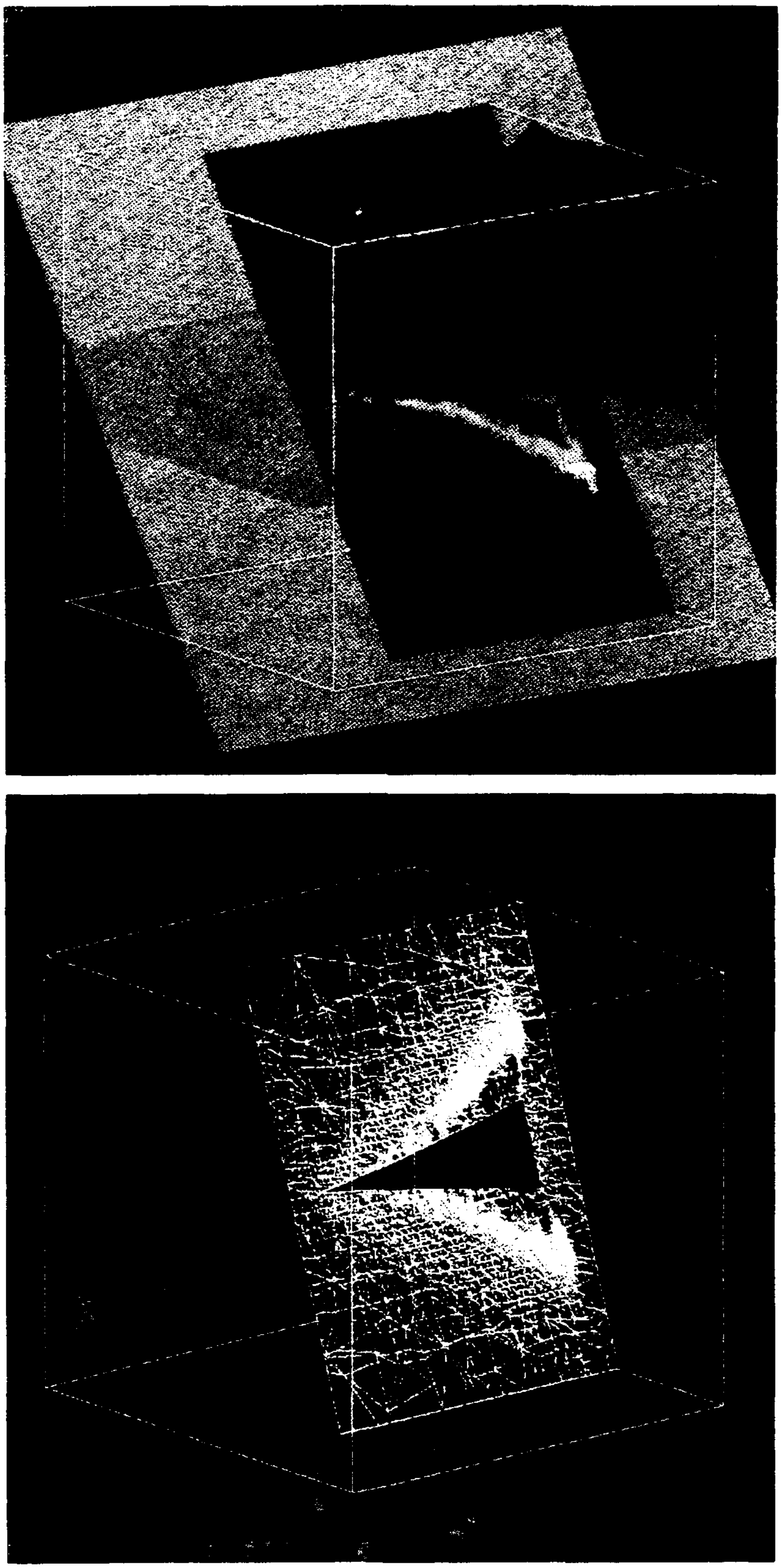

Figure 7. Shock surface and pressure contours found when computing the Mach two flow past a cone having a half angle of 10°.

2. Interactions.

Key invited lectures by J. E. Flaherty on material connected with the research supported by this grant are listed below. (Invited university colloquia are only presented for the last twelve months.)

1. "Adaptive Methods and Parallel Computation for Partial Differential Equations," Special Session on Adaptive Methods at the *Eighth Army Conference on Applied Mathematics and Computing*, Cornell University, Ithaca, June 19-22, 1990.

2. "Symbolic and Parallel Adaptive Methods for Partial Differential Equations," *Workshop on the Integration of Numerical and Symbolic Computing Methods*, Saratoga Springs, July 8-11, 1990.

3. "Advances in Parallel Processing for Electromagnetic Field Applications," *Fourth Biennial IEEE Conference on Electromagnetic Field Computation*, Toronto, October 22-24, 1990.

4. "Adaptive Finite Element Schemes for Parabolic Partial Differential Systems with H-, P-, and R-Refinement," *AICHE Annual Meeting*, Chicago, November 12-16, 1990.

5. "Combined Symbolic and Numerical Adaptive Methods for Partial Differential Equations," *Workshop on Problem Solving Environments*, National Science Foundation, Washington, April 11-12, 1991.

6. "Adaptive Methods for PDEs," Conference on *Experimental Mathematics: Computational Issues in Nonlinear Science*, Los Alamos National Laboratory, Los Alamos, May 20-24, 1991.

7. "Adaptive h- and p-Refinement Finite Element Methods for Singularly Perturbed Parabolic Systems," *ICIAM 91*, Minisymposium on "Numerical Methods for Singularly-Perturbed Problems," Washington, July 8-12, 1991.

8. "A Posteriori Error Estimation for Parabolic Systems" and "High-Order Adaptive Methods for Parabolic Systems," *First U. S. National Congress on Computational Mechanics*, Chicago, July 21-24, 1991.

9. "Parallel Adaptive Methods for Partial Differential Equations," *Workshop on Parallel Scientific Computation*, Rensselaer Polytechnic Institute, Troy October 31, November 1, 1991.

10. "Adaptive Method-of-Lines Techniques for Parabolic Systems," *First International Symposium on Method of Lines, Surfaces and Dimensional Reduction in Computational Mathematics and Mechanics*, Athens, November 12-16, 1991.

11. "High-Order Adaptive Methods for parabolic and Elliptic Systems," New Jersey Institute of Technology, Newark, April 20, 1992.

12. "Parallel Adaptive Techniques," *Workshop on Adaptive Methods for Partial Differential Equations,* Rensselaer Polytechnic Institute, Troy, May 17-20, 1992.

13. "Parallel High-Order Finite Element Methods for Conservation Laws," *IMACS Seventh Internation Conference on Computer Methods for Partial Differential Equations," New Brunswick, June 22-24, 1992.*

14. "Adaptive Methods for Time-Dependent Partial Differential Equations," *SIAM 40th Anniversary Meeting,* Los Angeles, July 20-24 1992.

15. "Adaptive Methods for Time-Dependent Partial Differential Equations," ICASE, NASA Langley Research Center, Hampton, July 23, 1992.

16. "Adaptive Methods for Time-Dependent partial Differential Equations. Part I: Basic Strategies and Error Estimation" and "Part II: High-Order Methods and Parallel Computation," *Dutch Numerical Analysis Seminar,* Woudschoten Conference Center, Zeist, October 5-7, 1992.

17. "High-Order Adaptive Methods for Time-Dependent Partial Differential Equations," Washington University, St. Louis, October 29, 1992.

18. "Coloring Procedures for Finite Element Computation on Shared-Memory Computers," Symposium on *Adaptive, Multilevel, and Hierarchical Computational Strategies,* ASME Winter Annual Meeting, Anaheim, November 8-13, 1992.

19 "Adaptive and Parallel High-Order Methods for Conservation Laws," Mississippi State University, Mississippi State, January 22, 1993.

20. "Adaptive and Parallel High-Order Methods for Conservation Laws," University of Texas, Austin, March 13-22, 1993.

21. "Adaptive and Parallel High-Order Methods for Conservation Laws," University of Kentucky, Lexington, April 21, 1993.

22. "Adaptive hp-Refinement Methods for Parabolic Partial Differential Equations," *1993 AFOSR Workshop on Computational Mathematics,* Washington University, St. Louis, May 19-21, 1993.

Other interactions follow.

1. J. E. Flaherty and B. K. Szymanski organized a workshop on *Parallel Scientific Computation* which was held at the Rensselaer Polytechnic Institute, October 31 and November 1, 1991.

2. J. E. Flaherty and M. S. Shephard, organized the *Workshop on Adaptive Methods for Partial Differential Equations* which was held at the Rensselaer Polytechnic Institute, Troy, May 17-20, 1992.

3. J. E. Flaherty organized a special session on *Adaptive Methods for Time-Dependent and Nonlinear Partial Differential Systems* which was held at the *IMACS Seventh Internation Conference on Computer Methods for Partial Differential Equations,"* New Brunswick, June 22-24, 1992.

4. Lenart Johnson of Thinking Machines Corporation visited J. E. Flaherty at Rensselaer on September 10, 1992. Flaherty and graduate student Raymond Loy visited Johnson, Zdenek Johann, et al. at Thinking Machines on March 3, 1993. Both visits involved discussions of parallel adaptive techniques for partial differential equations.

5. L. R. Petzold of the University of Minnesota visited J. E. Flaherty on September 30, 1992 to present a colloquium and discuss research on parallel adaptive techniques for partial differential equations.

6. J. E. Flaherty attended the *AFOSR Electronic Prototyping Initiative Review Meeting* at the University of Michigan, Ann Arbor, May 27, 1993.

3. Publications and Manuscripts

Publications

1. D.C. Arney and J.E. Flaherty, "An Adaptive Mesh Moving and Local Refinement Method for Time-Dependent Partial Differential Equations," *ACM Trans. Math. Software,* **16** (1990), pp. 48-71.

2. P.K. Moore and J.E. Flaherty, "A Local Refinement Finite Element Method for One-Dimensional Parabolic Systems," *SIAM J. Numer. Anal.,* **27** (1990), pp. 1422-1444.

3. M. Benantar, R. Biswas, J.E. Flaherty, and M. S. Shephard, "Parallel Computation with Adaptive Methods for Elliptic and Hyperbolic Systems," *Comp. Meths. Appl. Mech. and Engrg.,* **82** (1990), pp. 73-93.

4. P.K. Moore and J.E. Flaherty, "Adaptive Local Overlapping Grid Methods for Parabolic Systems in Two Space Dimensions," *J. Comp. Phys.,* **98** (1992), pp. 54-63.

5. D.C. Arney, R. Biswas, and J.E. Flaherty, "An Adaptive Mesh Moving and Refinement Procedure for One-Dimensional Conservation Laws," *Appl. Numer. Math.,* **11** (1993), pp. 259-282.

6. M. Benantar and J.E. Flaherty, "A Six-Color Procedure for the Parallel Solution of Elliptic Systems Using the Finite Quadtree Structures," in J. Dongarra, P. Messing, D.C. Sorensen, and R.G. Voigt, Eds., *Proc. Fourth SIAM Conf. Parallel Proc. for Sci. Comput.,* **23** (1990), pp. 231-236.

7. J.E. Flaherty, M. Benantar, R. Biswas, and P.K. Moore, "Symbolic and Parallel Adaptive Methods for Partial Differential Equations," Chap. 12 in B.R. Donald, D. Kapur, and J.L. Mundy, Eds., *Symbolic and Numerical Computation for Artificial Intelligence,* Academic Press, London, pp. 277-302, 1992.

8. J.E. Flaherty and Y.J. Wang, "Experiments with an Adaptive h-, p-, and r-Refinement Finite Element Method for Parabolic Systems," in G.D. Byrne and W.E. Schiesser, Eds., *Recent Developments in Numerical Methods and Software for ODEs/DAEs/PDEs,* World Scientific, Singapore, pp. 55-80, 1992.

9. R. Biswas, M. Benantar, and J.E. Flaherty, "Adaptive Methods and Parallel Computation for Partial Differential Equations," *Trans. Eighth Army Conf. on Applied Maths. and Comput., ARO Report 91-1,* U.S. Army Research Office, Research Triangle Park, pp. 531-552, 1991.

10. M. Benantar, R. Biswas, and J.E. Flaherty, "Advances in Adaptive Parallel Processing for Field Applications," *IEEE Trans. Magnetics,* **27** (1991), pp. 3768-3773.

11. S. Adjerid, J.E. Flaherty, and Y.J. Wang, "A Posteriori Error Estimation with Finite Element Methods of Lines for One-Dimensional Parabolic Systems," *Numer. Math.*, **65** (1993), pp. 1-21.

12. S. Adjerid, J.E. Flaherty, P.K. Moore, and Y.J. Wang, "High-Order Adaptive Methods for Parabolic Systems," *Physica D*, **60** (1992), pp. 94-111.

13. B.E. Webster, M.S. Shephard, Z. Rusak, and J.E. Flaherty, "An Adaptive Finite Element Methodology for Rotorcraft Aerodynamics," in R. Vichnevetsky, D. Knight, and G. Richter, Eds. *Advances in Computer Methods for Partial Differential Equations - VII*, IMACS, New Brunswick, pp. 799-805, 1992.

14. R. Biswas and J.E. Flaherty, "Parallel and Adaptive Methods for Hyperbolic Partial Differential Equations," in R. Vichnevetsky, D. Knight, and G. Richter, Eds., *Advances in Computer Methods for Partial Differential Equations - VII*, IMACS, New Brunswick, pp. 67-74, 1992.

15. K.D. Devine and J.E. Flaherty, "Parallel High-Order Finite Element Methods for Conservation Laws," in R. Vichnevetsky, D. Knight, and G. Richter, Eds., *Advances in Computer Methods for Partial Differential Equations - VII*, IMACS, New Brunswick, pp. 202-208, 1992 (with K. D. Devine).

16. Y.J. Wang and J.E. Flaherty, "An Adaptive hp-Refinement Finite Element Method for Two-Dimensional PDEs," in R. Vichnevetsky, D. Knight, and G. Richter, Eds., *Advances in Computer Methods for Partial Differential Equations - VII*, IMACS, New Brunswick, pp. 788-793, 1992.

17. M. Benantar, J.E. Flaherty, and M.S. Krishnamoorthy, "Coloring Procedures for Finite Element Computation on Shared-Memory Parallel Computers," in A.K. Noor, Ed., *Adaptive, Multilevel, and Hierarchical Computational Strategies*, AMD Vol. 157, ASME, New York, pp. 435-490, 1992.

Manuscripts In Press

18. P.K. Moore and J.E. Flaherty, "High-Order Adaptive Finite Element-Singly Implicit Runge-Kutta Methods for Parabolic Differential Equations," *BIT*, to appear, 1993.

19. S. Adjerid, J.E. Flaherty, and Y.J. Wang, "Adaptive Method-of-Lines Techniques for Parabolic Systems," Proc. *First International Symposium on Method of Lines, Surfaces and Dimensional Reduction in Computational Mathematics and Mechanics*, 1993, to appear.

20. A.C.M. Moraes, J.E. Flaherty, and H. T. Nagamatsu, "Compressible Laminar Boundary Layers for Perfect and Real Gases in Equilibrium at Mach Numbers to 30," AIAA Paper 92-0757, *Thirtieth Aerospace Sciences Meeting and Exhibit*, Reno, Jan.

6-9, 1992. Also, submitted for publication.

21. M. Benantar, J.E. Flaherty, and M.S. Krishnamoorthy, "Triangle Graphs," submitted for publication, 1992.

22. R. Biswas, K.D. Devine, and J.E. Flaherty, "Parallel Adaptive Finite Element Methods for Conservation Laws," Tech. Rep. 93-5, Dept. Comp. Sci., Rensselaer Polytechnic Institute, 1993. Also, *Applied Numerical Mathematics,* to appear.

23. A.C.M. Moraes, J.E. Flaherty, and H.T. Nagamatsu, "A Finite Element and Symbolic Method for Studying Laminar Boundary Layers of Real Gases in Equilibrium at Mach Numbers to 30," submitted for publication, 1993.

24. K.D. Devine, J.E. Flaherty, S. Wheat, and A.B. Maccabe, "A Massively Parallel Adaptive Finite Element Method with Dynamic Load Balancing," Tech. Rep. SAND93-0936C, Sandia National Laboratories, 1993. Also, submitted for publication.

25. J.E. Flaherty and P.K. Moore, "An hp-Adaptive Method in Space and Time for Parabolic Systems," Tech. Rep. 93-15, Dept. Comp. Sci., Rensselaer Polytechnic Institute, 1993. Also, submitted for publication.

4. Ph.D. Graduates

The following individuals received partial support from this grant while Ph.D. students and graduated during the period covered by this report.

1. Raymond Schmidt, *Adaptive Quadtree Discretization for Fluid Flow Problems*, 1991, Mathematics, Rensselaer Polytechnic Institute. Currently: Research Associate, School of Management, Rensselaer Polytechnic Institute.

2. Yun J. Wang, *An Adaptive Local HPR-Refinement Finite Element Method for Parabolic Partial Differential Equations*, 1991, Mathematics, Rensselaer Polytechnic Institute. Currently: Postdoctoral Fellow, Computer Science, Rensselaer Polytechnic Institute.

3. Rupak Biswas, *Parallel and Adaptive Methods for Hyperbolic Partial Differential Systems*, 1991, Computer Science, Rensselaer Polytechnic Institute. Currently: Postdoctoral Fellow, Research Institute for Advanced Computer Science, NASA Ames Research Center.

4. Messaoud Benantar, *Parallel and Adaptive Algorithms for Elliptic Partial Differential Systems*, 1992, Computer Science, Rensselaer Polytechnic Institute. Currently: Enterprise Systems Division, IBM.

5. J. Michael Coyle, *An hr-Refinement Finite Element Method for Systems of Parabolic Partial Differential Equations with Stability Analyses for Mesh Movement*, 1993, Mathematics, Rensselaer Polytechnic Institute. Currently: Mathematician, Benét Laboratories.